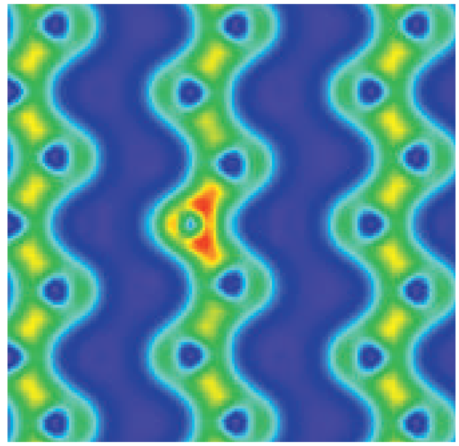
Massively Parallel Computing CRADA



Contours of electronic charge density for a boron impurity atom substituting for one silicon atom in a silicon crystal. The pileup of charge (red) around the boron atom suggests the formation of strong ionic bonds with the neighboring silicon atoms.

IN the most far-reaching technology transfer initiative to date, the Laboratory is working with industry to develop software for massively parallel supercomputers. In June 1994, Secretary of Energy Hazel O'Leary announced a $66 million joint venture involving LLNL, Los Alamos National Laboratory, and an industry group headed by Cray Research, Inc. The three-year, cost-sharing agreement, called the High-Performace Parallel Processing Project, involves Cray Research and 16 other leading industrial firms.

In one part of this endeavor, the consortium will develop software for high-performance parallel processing systems to be used in industrial applications, such as environmental modeling, materials design, and advanced manufacturing. The overall initiative, called the Industrial Computing Initiative, involves some 15 separate CRADAs. One of these projects, which teams LLNL with Xerox Corporation's Palo Alto Research Center and Cray Research, is focused on advanced atomic-level materials design. The primary objective of this project is to apply advanced *ab initio* electronic structure methods to specific physics problems of importance to research activities at Xerox, including investigations of the atomic and electronic structure of amorphous silicon and defect energetics in semiconductor materials.

To accomplish the goals of the projects, the DOE has leased two 128-processor Cray T3D massively parallel computers—one to Los Alamos and the other to the newly formed Center for Computing Sciences and Engineering at LLNL. The two T3Ds will be linked by a high-speed interconnect for collaborative work. These T3Ds can operate at peak speeds of 18 billion floating point operations per second (18 Gflops), which is comparable to the fastest vector supercomputer now at the Laboratory, but a T3D is only about one-tenth the purchase cost.

Much of the software for existing supercomputers was originally developed by the DOE laboratories for their national security missions. However, atomic-level materials modeling also benefits the economic competitiveness of the nation by focusing on industrial problems. The software that industry needs is difficult to write or upgrade from serial to parallel-style codes. New software from the Industrial Computing Initiative will help the private sector make the transition to massively parallel systems, aid industry in designing better materials, and help companies insert new products into the market faster.

Our work with Xerox and Cray Research is aimed at developing codes that simulate materials at the atomic level from first-principles, quantum-mechanical methods. Material properties—whether optical, structural, or electrical—are ultimately determined by electronic structure. The codes developed during this CRADA will extend the Laboratory's current electronic-structure codes to exploit the potential of massively parallel computers. The new capability will allow us to routinely calculate electronic structure in much larger systems and with greater accuracy than was ever possible before.

For example, the figure shows contours of electron charge density for a boron impurity atom substituting for one silicon atom in a silicon crystal. The pileup of charge (red) around the boron atom suggests the formation of strong ionic bonds with the neighboring silicon atoms. Research on defects and impurities in semiconductors will help scientists synthesize materials such as gallium arsenide and amorphous silicon. Gallium arsenide is a light-emitting semiconductor used in the diode laser found in laser printers. Amorphous silicon is used in imaging and scanning devices and in thin-film transistors that are part of flat-panel displays. Research on this and related materials could lead to a new generation of transistors in flat-panel displays for laptop computers, an area in which Japan has a dominant lead over U.S. companies.

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